

Non-extensive statistical mechanics: Gibbs-type formula, existence and uniqueness of its solution

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Abstract

Existence and uniqueness results for the solution of the Gibbs-type formula from non-extensive mechanics are derived rigorously. A new conditional extremal problem is proposed to get in a more simple way the Gibbs-type formula itself.

1 Introduction

Non-extensive statistical mechanics is an actively studied domain and a spacious bibliography exists already (see some references in [1, 8, 9]). Following C. Tsallis [8] we define entropy by a basic formula from non-extensive mechanics:

$$S_q = (1 - \sum_{i=1}^n p_i^q)/(q - 1), \quad \sum_{i=1}^n p_i = 1, \quad p_i > 0, \quad q > 0, \quad (1)$$

where n is the total number of probabilities. Energy is defined by the formula (see[8]):

$$U_q = (\sum_{i=1}^n p_i^q E_i)/(\sum_{i=1}^n p_i^q), \quad (2)$$

where E_i are the eigenvalues of the Hamiltonian of the corresponding system. In our approach we consider a new extremal problem. Namely, we fix the

Lagrange multiplier $\beta = 1/kT$, that is, we fix the temperature and introduce the Helmholtz free energy (up to a constant multiple) as the compromise function

$$F(\beta, p_1, p_2, \dots, p_n) = -\beta U_q + S_q.$$

Similar to [5, 6] we assume the

Fundamental principle: *The probabilities $\{p_i\}$ are the coordinates of the stationary point of the compromise function.*

Hence, the probabilities $\{p_i\}$ and, correspondingly, the mean energy U_q and the entropy S_q are obtained as the solution of this extremal problem.

The suggested approach affords a simple and rigorous treatment of the basic Gibbs-type formula, being a development of the papers [5] and [6], where the same approach was applied to ordinary quantum and classical mechanics, respectively. Namely, we recall that the stationary point $\tilde{P} = (\tilde{p}_1, \tilde{p}_2, \dots, \tilde{p}_n)$ of the function $F(\beta, p_1, p_2, \dots, p_n)$ is a solution of the system

$$\frac{\partial F(\beta, p_1, p_2, \dots, p_n)}{\partial p_i} = 0, \quad 1 \leq i \leq n. \quad (3)$$

In view of (3), it is easy to see that the fundamental principle implies equalities

$$\tilde{p}_i = \hat{Z}_q^{-1} \left(1 + (q-1)\beta(E_i - U_q) / \left(\sum_{i=1}^n \tilde{p}_i^q \right)^{\frac{1}{1-q}} \right), \quad (4)$$

where

$$\hat{Z}_q = \sum_{i=1}^n \left(1 + (q-1)\beta(E_i - U_q) / \left(\sum_{i=1}^n \tilde{p}_i^q \right)^{\frac{1}{1-q}} \right). \quad (5)$$

Thus, the fundamental principle conforms to the basic Gibbs-type relations from [8, p. 12]. There is also an interesting intersection with the results from game theory, which is discussed in the Conclusion.

We note that (differently from the classical Gibbs formula) the Gibbs-type formula (4) is, in fact, an equation. Thus, an important problem of the existence and uniqueness of its solution appear. Further we denote probabilities satisfying fundamental principle and so satisfying (4) by \tilde{p}_i . The next section is dedicated to the rigorous proof of the existence and uniqueness of the solution of (4).

2 Extremum points

We introduce the following values

$$E_{\max} = \max\{E_1, E_2, \dots, E_n\}, \quad E_{\min} = \min\{E_1, E_2, \dots, E_n\}. \quad (6)$$

We need such a solution \tilde{p}_i of system (4), (5), that

$$\tilde{p}_i > 0, \quad 1 \leq i \leq n. \quad (7)$$

Proposition 2.1 *Let the following conditions*

$$q > 1, \quad \beta > 0, \quad 1 - \beta(q - 1)(E_{\max} - E_{\min})n^{q-1} > 0 \quad (8)$$

hold. Then every solution of system (4), (5) satisfies conditions (7).

Proof. The assertion of the proposition follows directly from (1.4), (1.5) and the inequality

$$z_q = \sum_{i=1}^n p_i^q \geq n^{1-q}.$$

■

Proposition 2.2 *Let the following conditions*

$$0 < q < 1, \quad \beta > 0, \quad 1 + \beta(1 - q)(E_{\min} - E_{\max}) > 0 \quad (9)$$

hold. Then every solution of system (4), (5) satisfies conditions (7).

Proof. The assertion of the proposition follows directly from (4), (5) and the inequality

$$z_q = \sum_{i=1}^n p_i^q \geq 1.$$

■

Remark 2.3 *Proposition 2.2 is true in the case $n = \infty$ as well.*

Let us denote by $D = \{(p_1, p_2, \dots, p_n)\}$ the set of points, where

$$p_i \geq 0, \quad 1 \leq i \leq n; \quad \sum_{i=1}^n p_i = 1. \quad (10)$$

The set D is compact and convex. A topological space X is said to have the fixed point property (briefly FPP) if for any continuous function $f : X \rightarrow X$ there exists $x \in X$ such that $f(x) = x$. According to the Brouwer fixed point theorem, every compact and convex subset of a euclidean space has the FPP.

It is easy to see, that the following statement is true.

Proposition 2.4 *Let the conditions of either Proposition 2.1 or Proposition 2.2 hold. Then the relations*

$$r_i = \hat{Z}_q^{-1} \left(1 + (q-1)\beta(E_i - U_q) / \left(\sum_{i=1}^n p_i^q \right)^{\frac{1}{1-q}} \right), \quad (11)$$

where

$$\hat{Z}_q = \sum_{i=1}^n \left(1 + (q-1)\beta(E_i - U_q) / \left(\sum_{i=1}^n p_i^q \right)^{\frac{1}{1-q}} \right), \quad (12)$$

continuously map the set D into itself.

Using Lefschetz fixed point theorem [2] we obtain the assertion:

Theorem 2.5 *Let relations (11) continuously map the set D into itself. Then there exists one and only one point*

$$\tilde{P} = (\tilde{p}_1, \tilde{p}_2, \dots, \tilde{p}_n),$$

which satisfies relations (4), (5), and $\tilde{P} \in D$.

Proof. It follows from the analyticity of r_i that the map under consideration has only a finite number N_f of fixed points. Hence we can apply the Lefschetz fixed point theorem [2]. According to this theorem the number N_f coincides with the Euler characteristics $\chi(D)$ of D . In view of the well-known Euler formula we have $\chi(D) = 1$. The theorem is proved. ■

Remark 2.6 *Relations (11) continuously map the set D into itself if either conditions of Proposition 2.1 or conditions of Proposition 2.2 are fulfilled.*

We stress, that we consider the extremal problem for the introduced function F , which contains the fixed parameter β , but the energy U_q is not fixed. The case, where the energy U_q is fixed, was treated in a number of works but the corresponding equation for the Lagrange multiplier is transcendental and very complicated.

For the proof of our next proposition, we use the classical iteration method and take $P_0 = (1/n, 1/n, \dots, 1/n)$ as the starting point.

Proposition 2.7 *If β is small, then*

$$\tilde{p}_i \approx 1/n + \beta(E_i - \bar{E})n^{-q}, \quad (13)$$

where $\bar{E} = (\sum_{i=1}^n E_i)/n$.

3 Conclusion

The traditional approach to entropy (and the importance of the rigorous treatment of this notion, wherever possible) was described by A. Wehrl [10] in the following statement: “*Traditionally entropy is derived from phenomenological thermodynamical considerations based upon the second law of thermodynamics. This method does not seem to be appropriate for a profound understanding of entropy*”.

In our note we address the problem of the rigorous treatment of the Gibbs-type formulas closely related to entropy. The conditional extremum problem that is treated in the note could be considered as the game situation in accordance with the definition that “*game theory models strategic situations in which an individual’s success in making choices depends on the choices of others*” (see, e.g., [3]).

The rigorous proof that under rather weak conditions the probabilities given by the Gibbs-type formula exist and are unique is both important and new.

The obtained results afford a rigorous treatment of other problems of non-extensive mechanics and applications to other domains (see, e.g., [4, 7]).

References

- [1] M. Gell-Mann and C. Tsallis (eds), *Nonextensive entropy – interdisciplinary applications* (Oxford University Press, New York, 2004).

- [2] S. Lefschetz, *Ann. Math.* (2) **38**, 819 (1937).
- [3] R. Myerson, *Game Theory: Analysis of Conflicts* (Harvard University Press, Cambridge, 1991).
- [4] L.A. Sakhnovich in: *Topics in operator theory*, J.A. Ball et al (eds), *Operator Theory: Advances and Applications* **202**, 489-495 (Birkhäuser, Basel, 2010).
- [5] L.A. Sakhnovich, *Physica A* **390**, 3679 (2011).
- [6] L.A. Sakhnovich, arXiv:1105.4633.
- [7] L.A. Sakhnovich, arXiv:1106.3254
- [8] C. Tsallis in: *Non-extensive Statistical Mechanics and Applications*, S. Abe and Y. Okamoto (eds), 3-98 (Springer, Berlin, 2001).
- [9] C. Tsallis, A.R. Plastino, and R.F. Alvarez-Estrada, *J. Math. Phys.* **50**, 043303, 12 p. (2009).
- [10] A. Wehrl, *Rev. Mod. Phys.* **50**, 221 (1978).